Nonuniversality in the pair contact process with diffusion

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Abstract

We study the static and dynamic behavior of the one dimensional pair contact process with diffusion. Several critical exponents are found to vary with the diffusion rate, while the order-parameter moment ratio $m = \overline{\rho^2}/\overline{\rho}^2$ grows logarithmically with the system size. The anomalous behavior of m is traced to a violation of scaling in the order parameter probability density, which in turn reflects the presence of *two distinct sectors*, one purely diffusive, the other reactive, within the active phase. Studies restricted to the reactive sector yield precise estimates for exponents β and $\nu_\perp$, and confirm finite size scaling of the order parameter. In the course of our study we determine, for the first time, the universal value $m_c = 1.334$ associated with the parity-conserving universality class in one dimension.

The pair contact process (PCP) [1,2] is a nonequilibrium stochastic model which, like the basic contact process (CP) [3–5], exhibits a phase transition to an absorbing state. While the absorbing state in the contact process corresponds to a unique configuration (an empty lattice), the PCP possesses infinitely many absorbing configurations. Numerical and theoretical studies nevertheless indicate that the PCP belongs to the same universality class as the CP (namely, that of directed percolation (DP)), but with anomalies in the critical spreading dynamics [1,2,6–12]. An infinite number of absorbing configurations arise in the PCP because all processes (creation and annihilation), require a nearest-neighbor (NN) pair of particles (to be referred to simply as a "pair" in what follows). If individual particles are allowed to hop on the lattice, however, there are but two absorbing states: the empty lattice, and the state of a single particle hopping.

Study of the diffusive pair contact process (PCPD) was stimulated by the observation of Howard and Täuber [13] that its Langevin description would involve complex noise (this in contradistinction to the CP and allied models (real noise) and the parity-conserving class (imaginary noise)). On the basis of numerical results in their pioneering density-matrix renormalization group study, Carlon et al. [14], noted that certain critical exponents in the PCPD had values similar to those known for the parity conserving (PC) universality class. Hinrichsen [15] reported simulation results inconsistent with the PCPD being in the parity conserving class, and instead proposed that the model defines a *distinct* class. In particular, while models in the PC class possess two symmetric absorbing states, the two absorbing states of the PCPD are not related by any symmetry. Interestingly, Park et al. found that even when such a symmetry is imposed on the PCPD, its critical exponents remain different from those of the PC class [16]. The distinctive behavior of the PCPD was further confirmed in simulations by Ódor [17], who presented evidence for the existence of two universality classes (for diffusion probabilities greater than, or less than, about 0.3). Henkel and Schollwöck, on the other hand, suggested, on the basis of a study of universal finite-size scaling amplitudes, that for finite diffusion rates, the critical behavior of the PCPD belongs to a single universality class [18]. Our goal in this Rapid Communication is to shed some light on this rather confusing situation by studying moment ratios and probability distributions in the critical PCPD.

The PCP is defined on a lattice, with each site either occupied (by a "particle") or vacant. Only pairs of occupied sites exhibit activity; each has a rate of p of mutual annihilation, and a rate of $1-p$ to create a new particle at a NN site, if this site (chosen at random) is vacant. For $p > p_c$ ($\simeq 0.077\ 090(5)$ in 1-d [6]), the system falls into the absorbing state (all activity ceases). The order parameter is the density of pairs.

In the PCPD, in addition to the creation and annihilation processes described above, each particle attempts to hop, at rate D, to a randomly chosen NN site; the move is accepted if the target site is vacant. The model again exhibits a continuous transition to the absorbing state, at a critical annihilation rate $p_c(D)$ that increases with the diffusion rate. Once particles are allowed to diffuse, the nature of the system changes radically. The absorbing state is modified as noted above, and the

order parameter is now the particle density not the pair density. In contrast to simpler models like the CP, in which diffusion does not alter the critical behavior [19,20], diffusion represents a *singular perturbation* in the pair contact process, since any $D > 0$ implies a fundamental change in the phase structure and in the identity of the order parameter.

We perform extensive simulations of the one-dimensional PCPD, using systems of L = 20, 40,...,1280 sites, with durations of 10^4 - 4×10^6 time steps, and sample sizes of 10^4 - 10^6 realizations. Initially all sites are occupied. We determine the mean particle density $\overline{\rho}$, and pair density $\overline{\rho_p}$, the moment ratio $m = \overline{\rho^2}/\overline{\rho}^2$, and the survival probability $P_s(t)$. (The overline denotes a stationary average.) The exponential decay of the latter permits us to determine the lifetime τ. We concentrate on the critical region, $p \simeq p_c(D)$.

Experience with absorbing-state phase transitons leads us to expect the following scaling properties at the critical point: $\overline{\rho} \sim L^{-\beta/\nu_\perp}$; $\tau \sim L^{\nu_{||}/\nu_\perp}$; and $m \to m_c$, a universal critical value [6]. We use power-law dependence of ρ on system size to determine the critical annihilation rate $p_c(D)$. For comparison we applied the same algorithm to the parity-conserving branching-annihilating random walk (BAW) model studied by Zhong and ben-Avraham [21].

Fig. 1 shows the scaling of the order parameter with system size, at the critical point, for the PCPD and the BAW; in the PCPD, $\beta/\nu_\perp$ decreases with increasing diffusion rate. (The fact that the data points for the PCPD with $D = 0.5$ and the BAW are nearly identical appears to be a coincidence, since the scaling of the relaxation time τ is quite different in the two cases.) Fig. 2 shows that while the moment ratio m attains a limiting value in the BAW model, it *grows* with L in the PCPD (roughly, $\sim \ln L$), a most unusual behavior. We find $m_c = 1.3340(4)$ for the BAW model, while $m_c = 1.1735(5)$ for the directed percolation class in 1+1 dimensions [6].

In models with an absorbing-state phase transition, the probability distribution for the order-parameter, $P(\rho; L)$ is expected to exhibit scaling at the critical point,

$$P(\rho; L) = \overline{\rho}\, \mathcal{P}(\rho/\overline{\rho}), \tag{1}$$

where $\mathcal{P}$ is a normalized scaling function, as was verified for the PCP without diffusion [2]. In the present case, the steady growth of m_c with system size implies that $P(\rho; L)$ does not obey scaling. The particle and pair probability distributions, shown (for $D = 0.1$) in Fig. 3, evidently do not scale. Instead, the most probable value of the particle number is always 2 (configurations with fewer than two particles are of course absorbing), and the overwhelmingly most probably number of pairs is *zero*, independent of system size. The distributions exhibit a tail that grows broader with increasing system size; these "tail events" are responsible for the observed critical behavior. The tails, which have a Gaussian form, again violate the scaling of Eq. (1). (The pair distribution exhibits a second maximum, away from $\rho_p = 0$, whose position increases slowly with system size, roughly as $L^{0.6}$.)

The particle and pair probability distributions confirm lack of scaling, and, perhaps more importantly, provide a clue to the enigmatic behavior of the process. In the PCP without diffusion, there is always at least one pair present in the active

state. But once we add diffusion, being in the active (i.e., non-absorbing) state implies that there are at least two particles, but not neccessarily any pairs. At p_c, the process apparently favors configurations with a small number of particles, but with no pairs. (For $D = 0.1$, for example, the probability of having no pairs remains at about 0.8 for the the system sizes studied here, and shows no sign of decreasing as L grows; for $D = 0.5$ this probability is about 0.58, and for $D = 0.85$, about 0.5.) While in this "purely diffusive" sector, the activity is that of a set of random walkers, but the particle number does not change, and critical fluctuations are not generated. From time to time the system ventures into the sector with a nonzero pair number (the "reactive sector"), and may there exhibit a burst of creation and annihilation reactions. We expect the latter activity to possess scale invariance at p_c. Thus the probability distribution may be seen as a superposition of distributions associated with the two sectors. In this light, lack of scaling is quite understandable. In the purely diffusive sector, the particle-number distribution is highly-peaked at $n = 2$, with (for $D = 0.1$) a mean value of about 3.5, independent of system size. (For $D = 0.5$ and 0.85, the mean particle number in the purely diffusive sector is about 3.2).

These observations motivate us to *exclude* the purely diffusive sector by studying properties *conditioned on having at least one pair* in the system. Note that this does not modify the dynamics of the system in any way; we simply restrict the averages to configurations having one or more pairs. Fig. 4 shows the order parameter distribution in the reactive sector, plotted in the reduced variables $\rho* = \rho/\overline{\rho}$ and $P^* = \overline{\rho}P$, for the same parameter values as in Fig. 3. The distribution now assumes a form very similar to that found in the nondiffusive PCP [2], with a maximum at a nonzero value of the order parameter, and shows evidence of scaling. Thus the behavior in the reactive sector is much closer that familiar from the contact process, the PCP, and related models with an absorbing state phase transition.

Closer examination reveals, however, that the scaling collapse is imperfect. Studies of larger systems confirm that the maximum of the scaled order parameter distribution gradually shifts to smaller values of ρ^*, and that the distribution becomes broader, with increasing L. (The latter is evident in the results for m discussed below.) While we do not claim to have a complete understanding of this "defect," a possible explanation is that for large L, configurations with but a single pair represent a system with only a small reactive region, the remainder residing in the purely diffusive sector. We defer a full investigation of this rather subtle question to future work.

Once we restrict the sample to the reactive regime, we eliminate a large source of uncertainty (i.e., the erratic switching between the two sectors), and are able to obtain more precise results. Using, as before, the criterion of power-law dependence of $\overline{\rho}$ on system size, we determine the critical parameter p_c and the ratio $\beta/\nu_\perp$ to good precision; these values are given in Table I. Restricting the averages to the reactive sector changes the value of p_c by 0.1% or less. There are more pronounced changes in $\beta/\nu_\perp$: without the restriction, we obtain 0.585, 0.50, and 0.465 for $D =$ 0.1, 0.5 and 0.85, respectively. (We regard these as poorer estimates, colored by the superposition of the two sectors. Note however that these values exhibit the same

trend - decreasing $\beta/\nu_\perp$ with increasing diffusion rate - as observed in the reactive sector.) Fig. 4 (inset) shows the critical moment ratio m_c versus system size, in the reactive sector. Its value is now comparable (for the system sizes studied here), to that for the DP and PC classes, but a slow growth (roughly linear in $\ln L$) is again evident. (Restricting the sample to configurations with two pairs leads to a reduction in m, but not in its rate of growth with system size.)

A possible weak point in our analysis is that we assume finite size scaling (i.e., the power-law dependence of $\overline{\rho}$ on system size), in determining p_c, whilst the results for m indicate that there is still a (relatively weak) violation of scaling. We therefore check our method by studying the order parameter (again restricted to the reactive sector), in the supercritical regime, $p < p_c$. We verify that the order parameter follows a power law, $\overline{\rho} \sim (p_c - p)^\beta$, and in so doing obtain the estimates for β given in Table I. This exponent decreases steadily with D, as found in Ref. [17]. (A direct comparison with the results of Ref. [17] is not possible since the latter study uses a parallel-update scheme, in contrast to the sequential updating used here.)

In fact, our results verify finite size scaling for the order parameter, i.e., the relation,

$$\overline{\rho} = L^{-\beta/\nu_\perp} \mathcal{R}(L^{1/\nu_\perp} \Delta), \tag{2}$$

where $\Delta = p_c - p$ and the scaling function $\mathcal{R}(x) \sim x^\beta$ for $x \gg 1$. The data collapse is evident in Fig. 5. From this analysis we obtain $\nu_\perp = 1.10$, 1.09, and 1.10 for $D = 0.1$, 0.5 and 0.85, respectively, suggesting that this exponent does not vary with the diffusion rate.

We also studied the decay of the particle density starting from a fully occupied lattice at the critical point, restricting the sample to the reactive sector. (In the early stages of the evolution, the probability for the system to be in the reactive sector is nearly unity, but at later times this probability decays much more rapidly than the survival probability itself.) From a data-collapse analysis of $\rho(t)$, using the finite-size scaling form, $\rho = L^{-\beta/\nu_\perp} \mathcal{F}(t/L^{\nu_{||}/\nu_\perp})$, we obtain the estimates for $z = \nu_{||}/\nu_\perp$ listed in Table I. (The corresponding estimates, without the restriction to the reactive sector are: 1.87(1) for $D = 0.1$, 1.82(1) for $D = 0.5$ and 0.85.)

We complement our analysis with a study of dynamic properties, using a parallel-update scheme. (Details of the method will be reported elsewhere [22].) We determine the exponent δ from the decay of the particle density, starting with all sites occupied: $\rho \sim t^{-\delta}$. The exponent η is determined from the growth in the number of active sites, starting from a single pair: $n(t) \sim t^\eta$. The results (based on samples of 10^4 realizations, for systems of 1280 sites, without restricting the sample to the reactive sector), shown in Table II, indicate that these exponents also depend on the diffusion rate, and again are very different from those of the BAW class. Our results for δ and η are similar to those obtained by Ódor [17], although a direct numerical comparison is not possible, owing again to differences in the updating scheme.

In summary, we have performed extensive studies of the PCPD, including the probability distributions for the order parameter and number of pairs. Our results clearly exclude the model from both the parity-conserving and the DP universality classes, supporting Hinrichsen's proposal that the model belongs to a distinct class.

The criticial exponents β, η and $\nu_{||}$ vary with the diffusion rate, while $\nu_{\perp}$ appears to be independent of this parameter. An interesting open question is whether the PCPD can be described by a single universality class (with unusually strong corrections to scaling yielding an apparent variation of critical exponents on D) [18], two distinct universality classes (one for high diffusion rates, the other for low, but finite D), as suggested by Ódor [17], or even exponents that vary continuously with D. Our data are not sufficient to distinguish between these hypotheses. We note, however, that we observe relatively little change in the exponent values for $D = 0.5$ and 0.85, compared with the changes between $D = 0.1$ and 0.5. A similar observation applies to the size dependence of m shown in Fig. 4.

The growth of the moment ratio m with system size signals a violation of scaling in the associated probability distribution, which we have argued is a consequence of there being two sectors, one reactive, the other purely diffusive, within the active phase. Restricting averages to the reactive sector, we find good evidence of finite size scaling of the order parameter, and a much weaker violation of scaling for the probability distribution. The question of how this remaining violation may be eliminated is an important subject for future investigation. We expect that decomposition of configuration space into sectors will prove useful in understanding other systems exhibiting bursts of activity separated by long quiescent periods.

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TABLES

D	p_c	$\beta/\nu_\perp$	β	$\nu_\parallel/\nu_\perp$
0	0.077090(5)	0.2523(3)	0.2765	1.577(4)
0.1	0.10648(3)	0.503(6)	0.546(6)	2.04(4)
0.5	0.12045(3)	0.430(2)	0.468(2)	1.86(2)
0.85	0.13003(1)	0.412(2)	0.454(2)	1.77(2)
BAW	-	0.497(5)	0.922(5)	1.74(1)

Table I. Static exponents for the PCPD and the BAW model; figures in parentheses denote uncertainties. BAW results from Ref. [21].

D	p_c	δ	η
0.2	0.28526(1)	0.223(1)	0.198(1)
0.6	0.19324(6)	0.212(5)	0.220(1)
BAW	-	0.286(2)	0.286(2)

Table II. Dynamic exponents for the PCPD and BAW model. BAW results from Ref. [21].

FIGURE CAPTIONS

FIG. 1. Particle density ρ versus system size at the critical point in the PCPD and the BAW model.

FIG. 2. Moment ratio m versus system size at the critical point in the PCPD and the BAW model.

FIG. 3. Probability distribution of the number of particles n for $D=0.1$. +: $L=80$; $\times$: $L=160$; $\Box$: $L=320$. The inset shows the corresponding probability distributions for the number of pairs, n_p. Note that the most probable value of n_p is zero.

FIG. 4. Scaling plot of the probability distribution in the reactive sector for the same parameter values as in Fig. 3. Inset: moment ratio m versus system size in the reactive sector; filled squares: $D=0.1$; +: $D=0.5$; $\times$: $D=0.85$.

FIG. 5. Scaling plot of the order parameter in the reactive sector for $D=0.1$. +: $L=640$; $\times$: $L=1280$; $\Box$: $L=2560$.

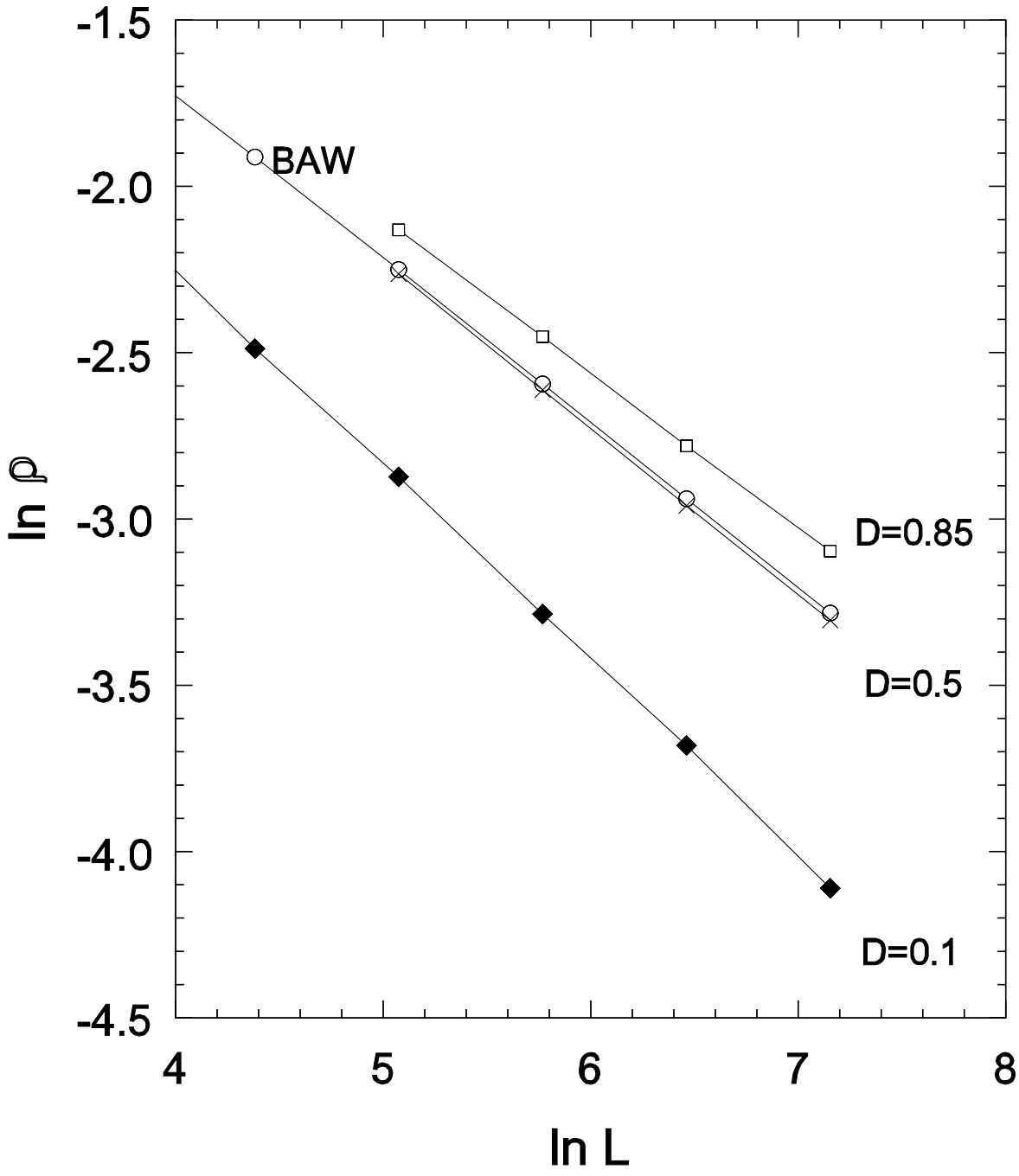


FIG. 1

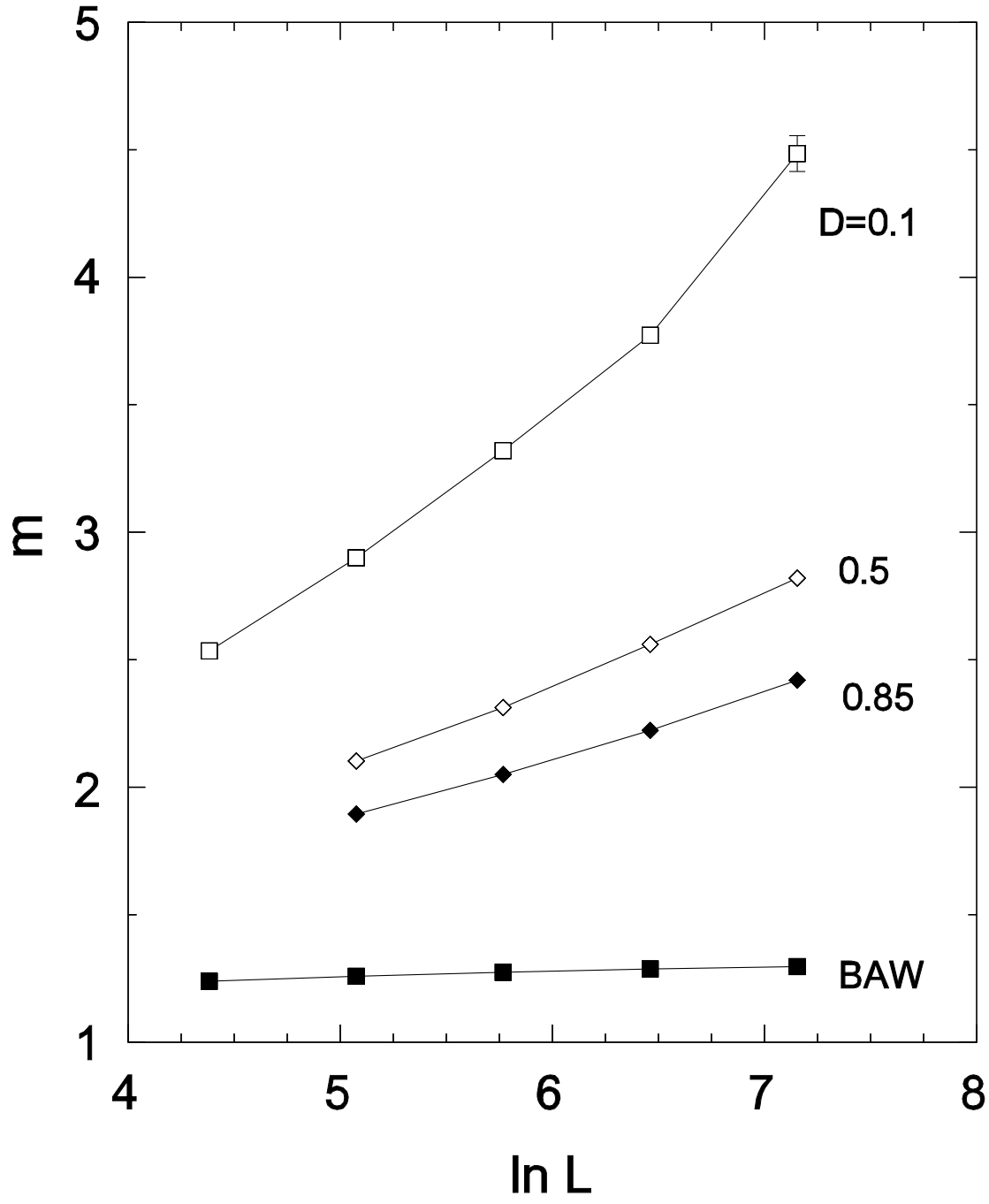
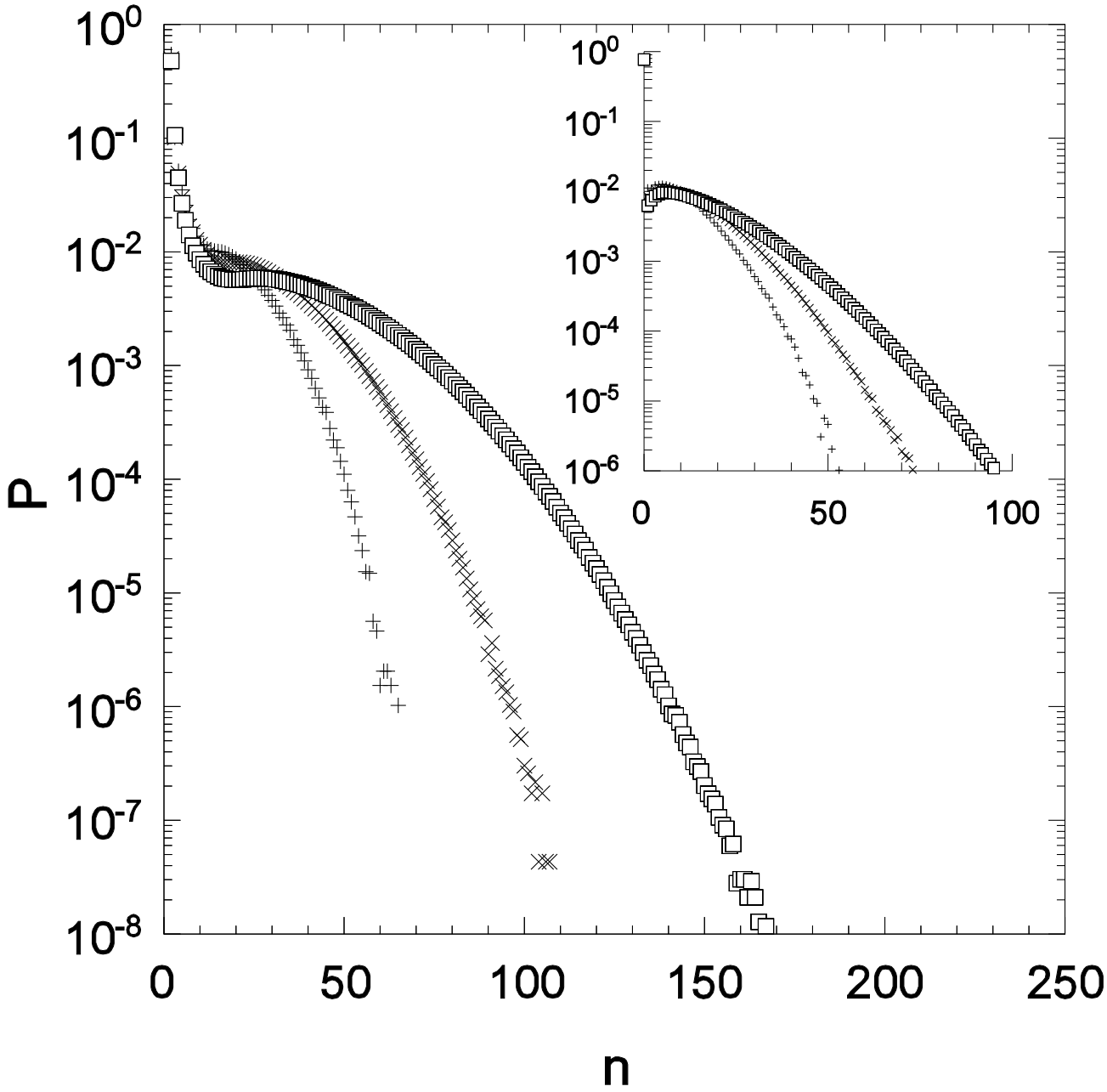


FIG. 2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50
100
150
200
250
10^{0}
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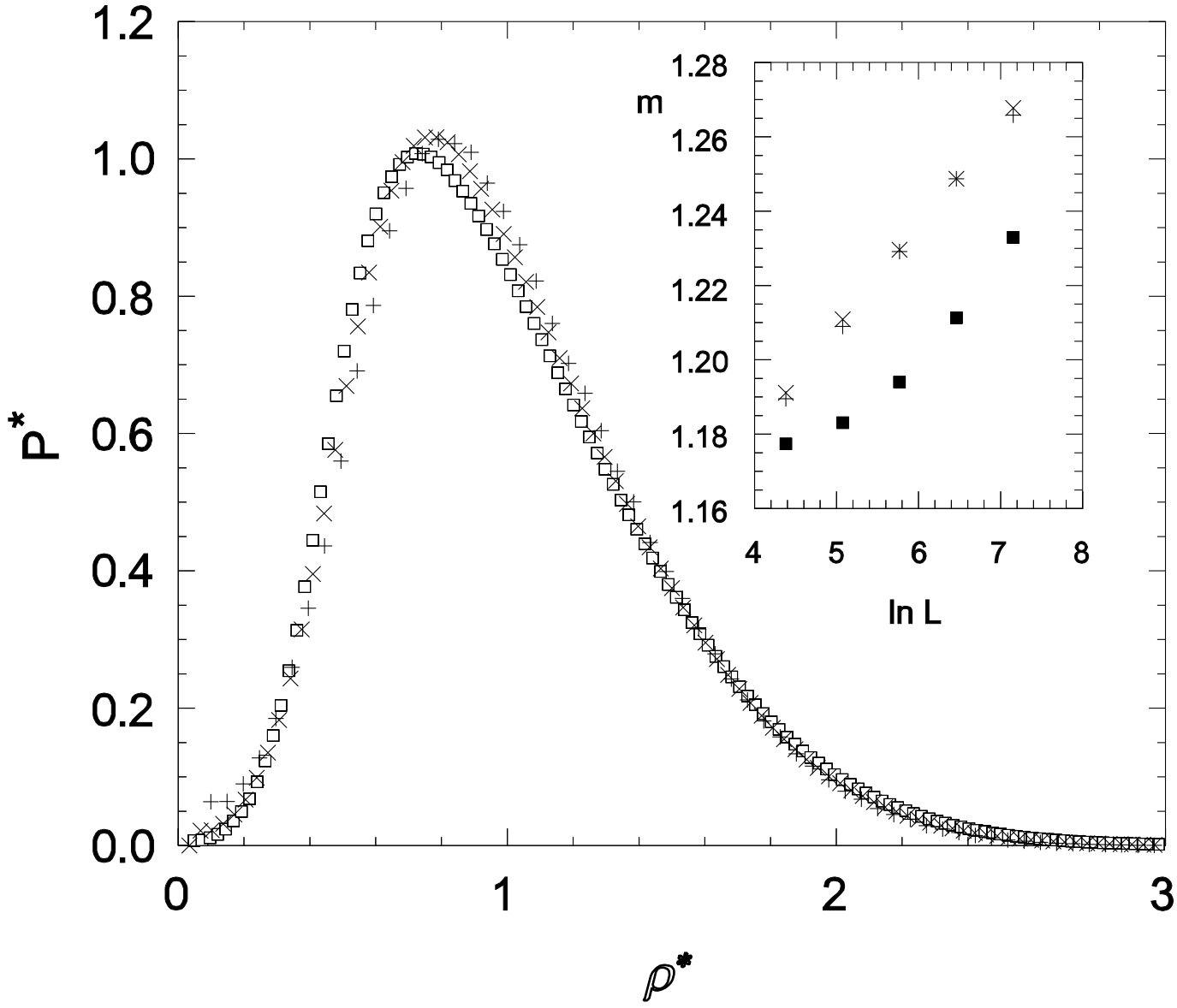
10^{-6}
0
50
100

FIG. 3


1.2
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0.8
0.6
0.4
0.2
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p^*
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1
2
3
ρ^*
m
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1.22
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7
8
ln L

FIG. 4

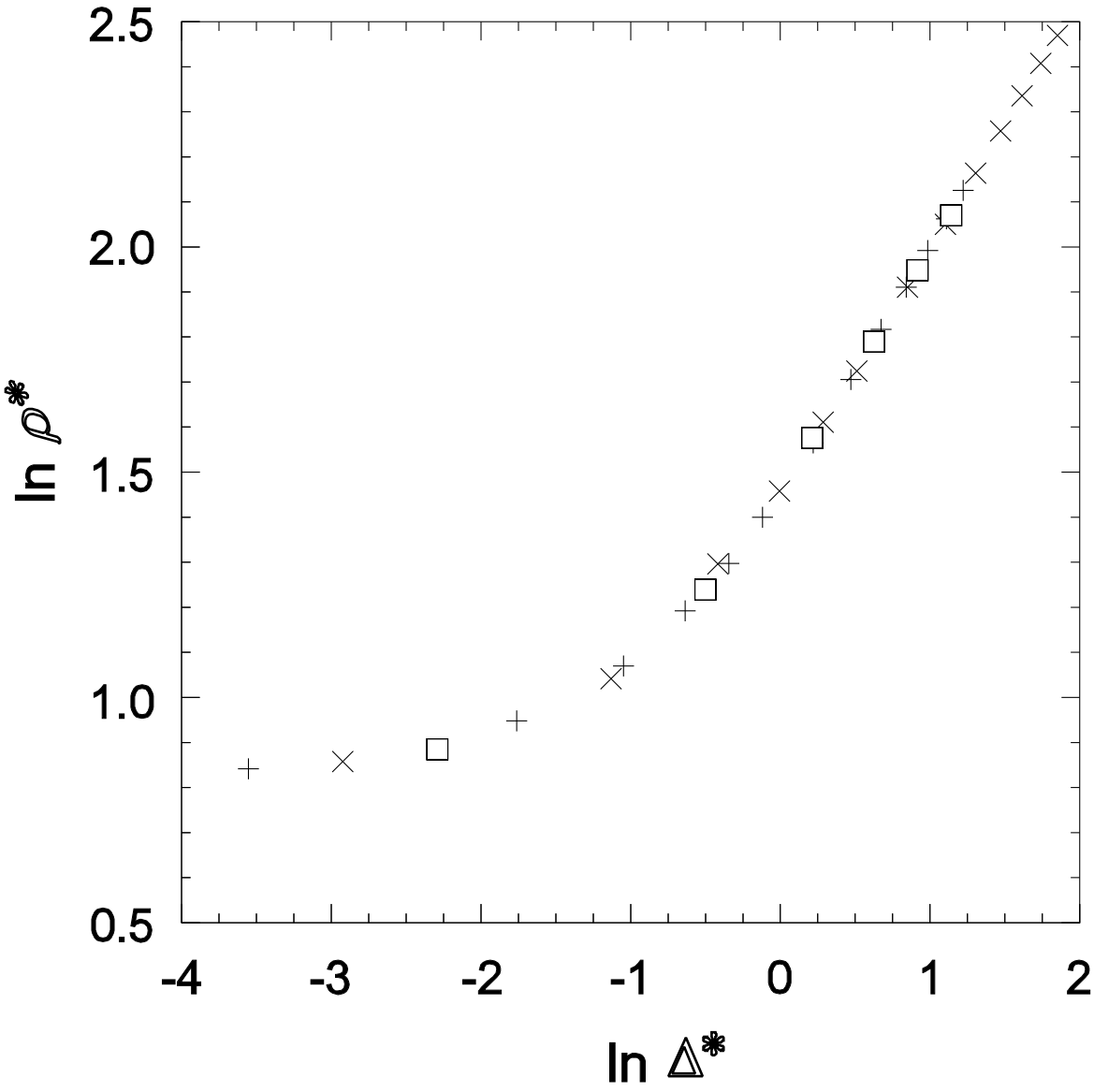

FIG. 5